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FIG. 1
Procedure for Modeling Complexes

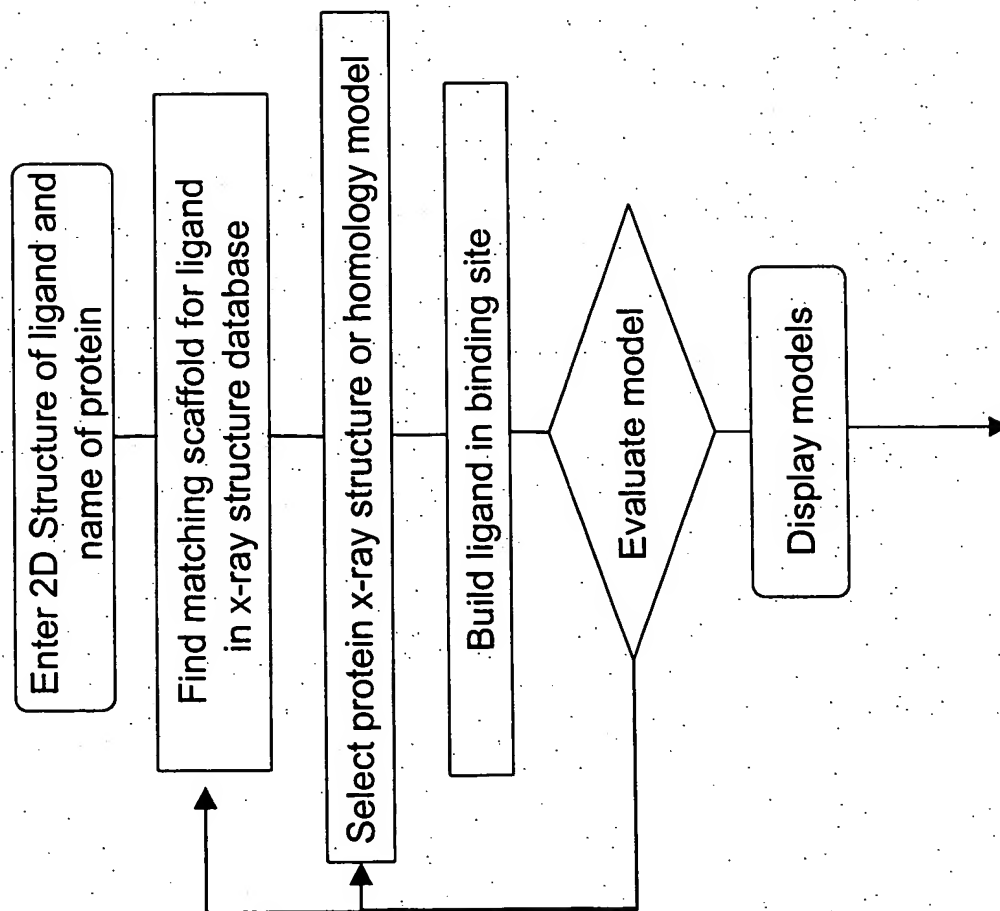


FIG. 2

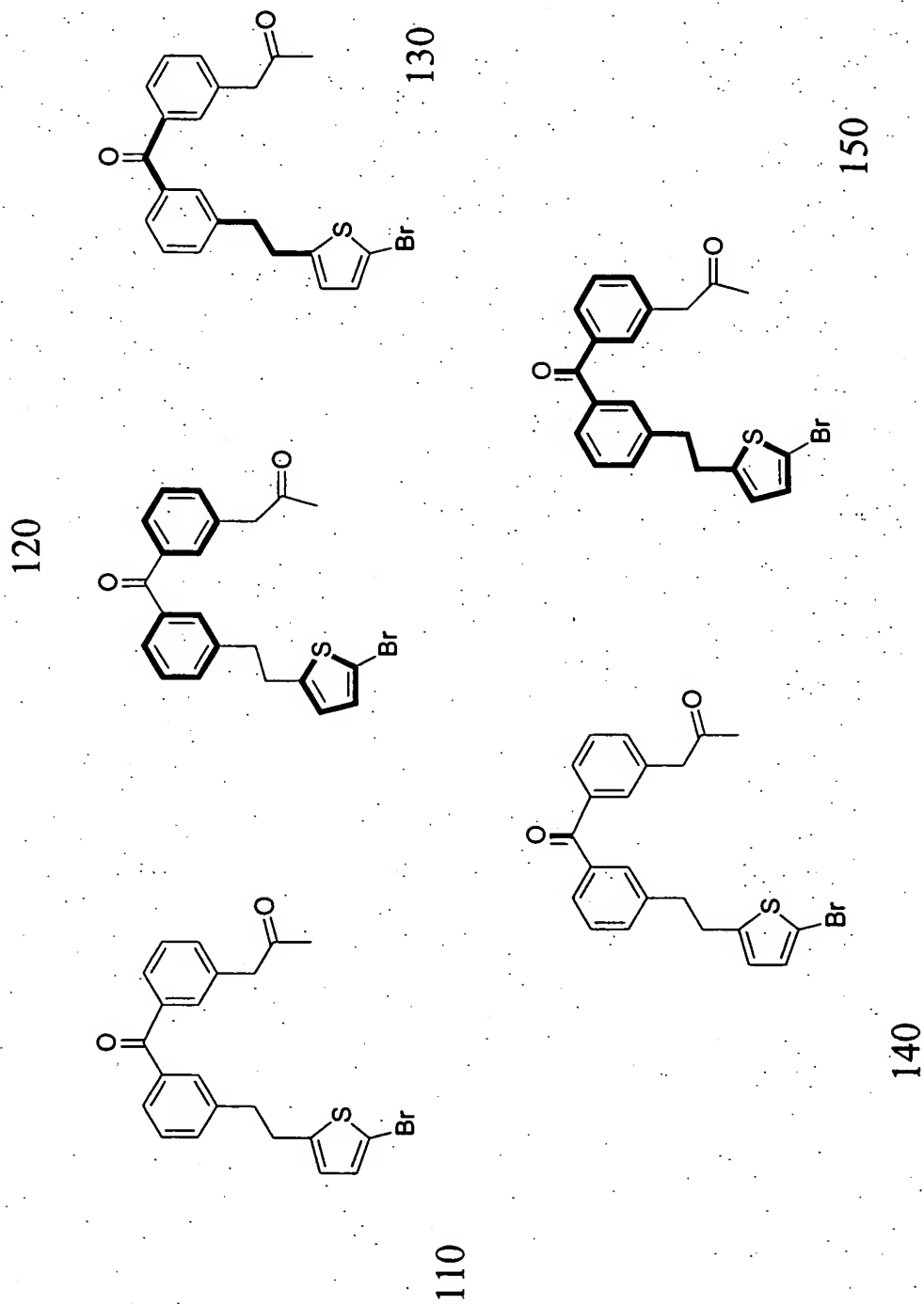


FIG. 3
Maximum Common Substructure

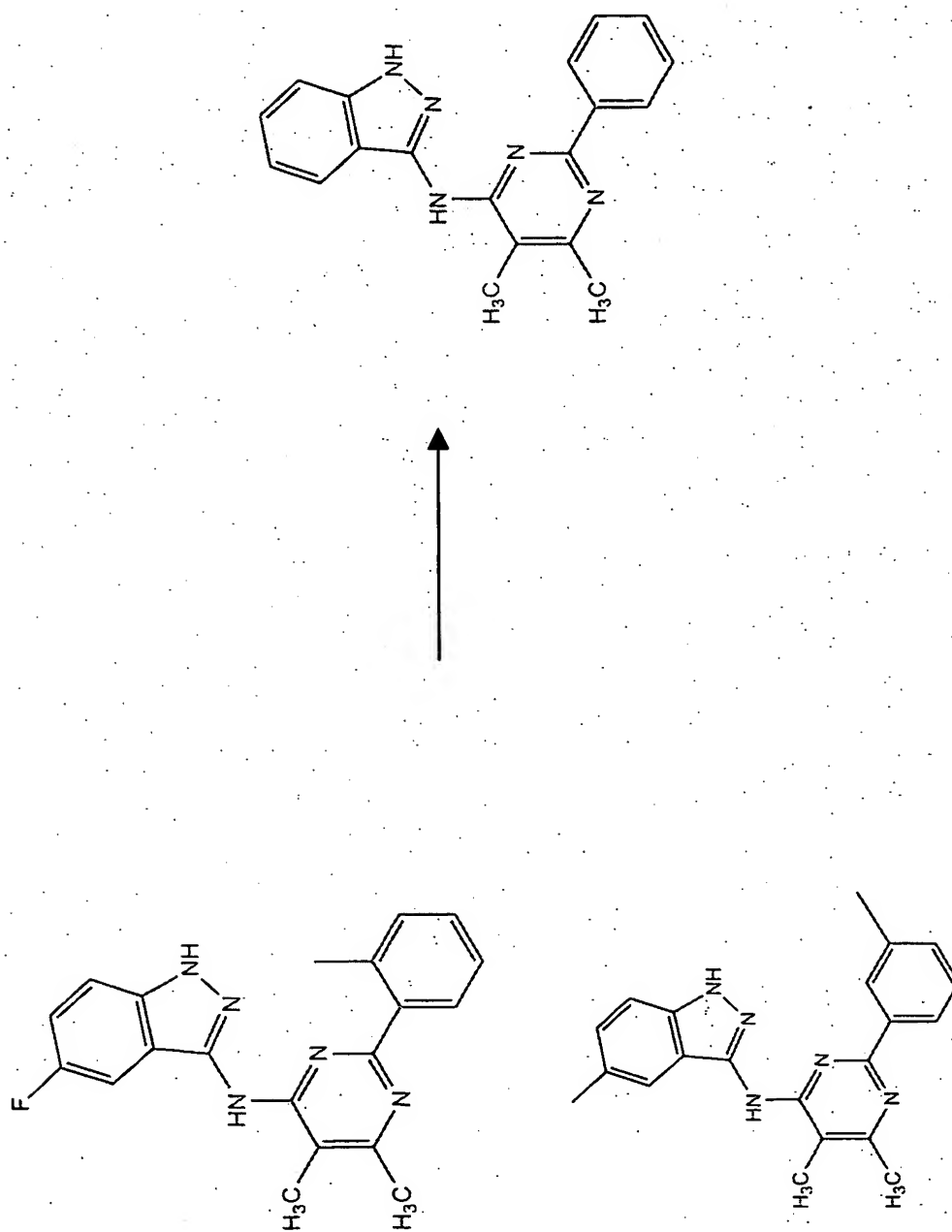
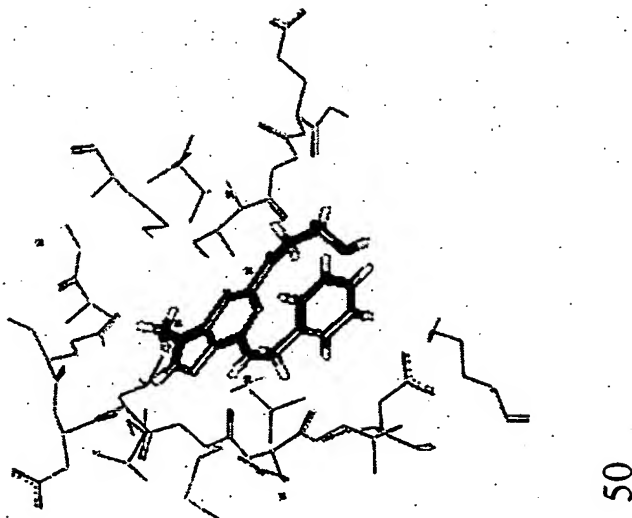
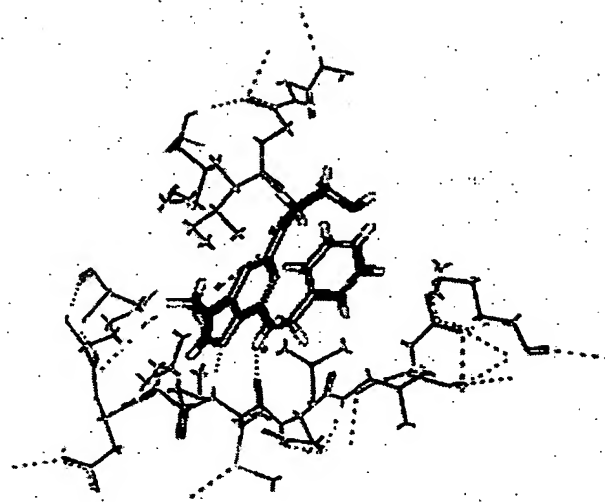


FIG. 4A



60



70

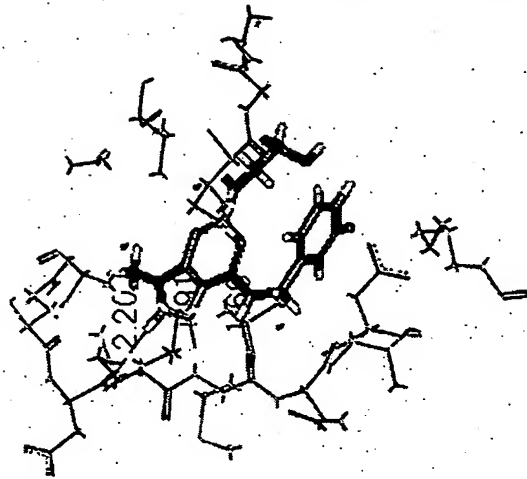
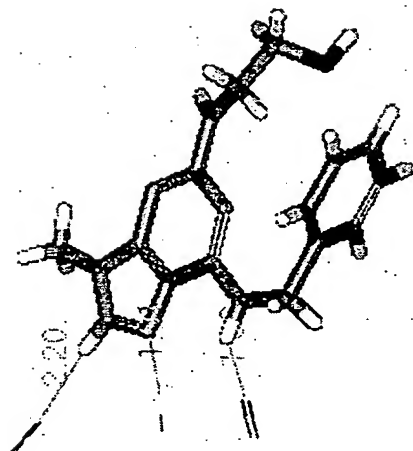
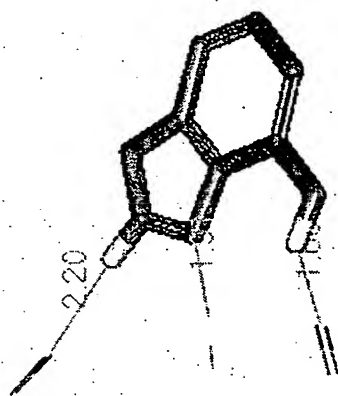


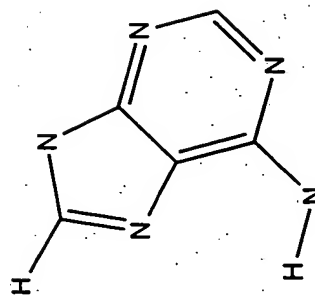
FIG. 4B



80



90



100

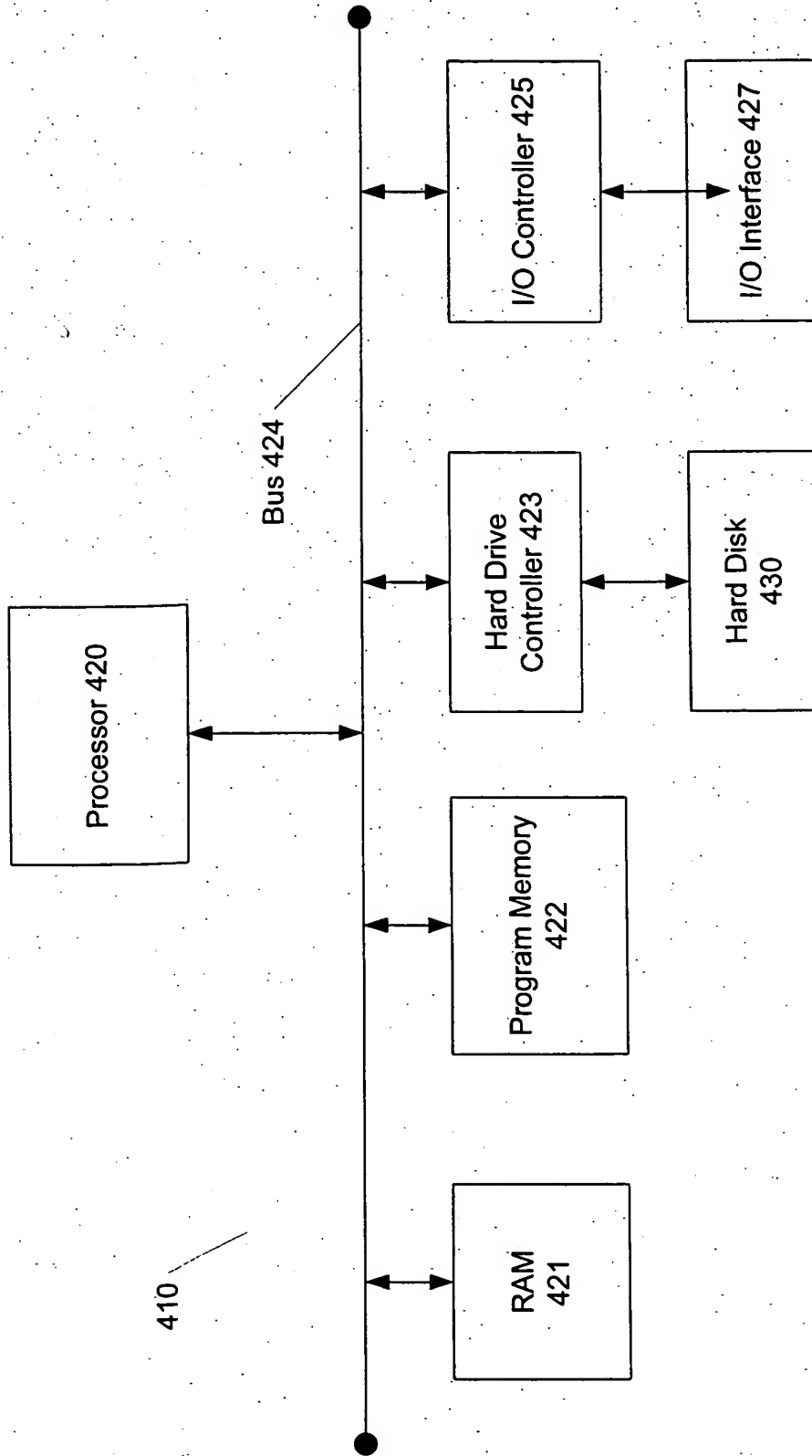


FIG. 5

FIG. 6

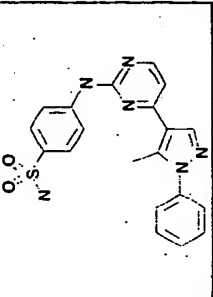
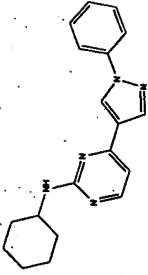
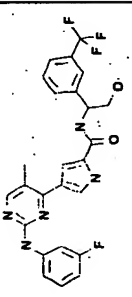
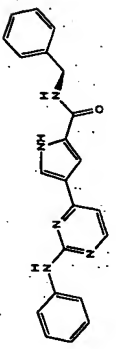
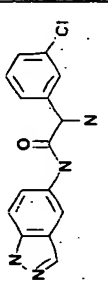
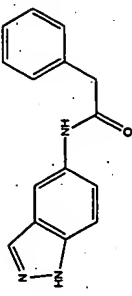
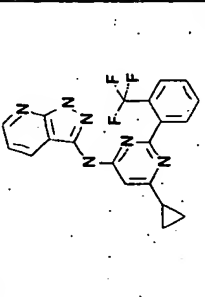
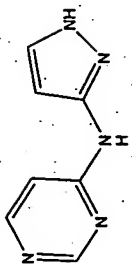
query ligand	protein	scaffold	rmsd (model vs. x-ray) / Angstrom
	jnk3		0.9 – 1.3
	erk2		1.5 – 2.0
	pka(5xm)		1.2
	gsk3β		1.3 – 2.2

FIG. 7A

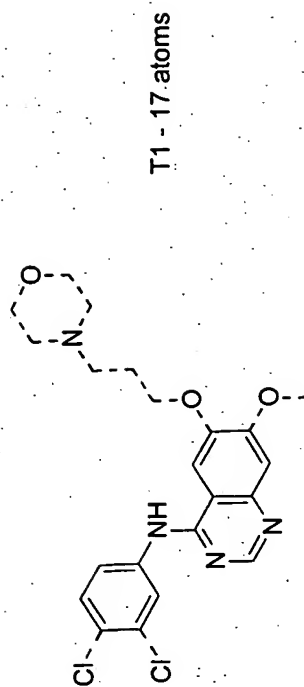


FIG. 7B

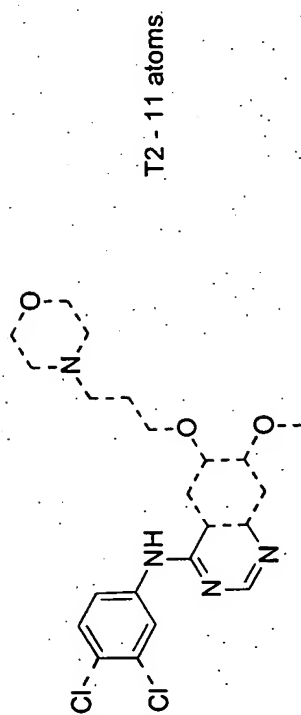


FIG. 7C

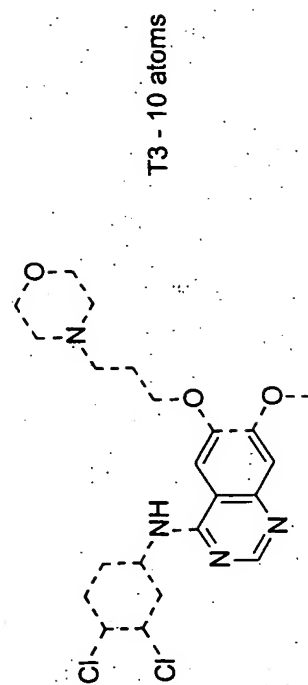
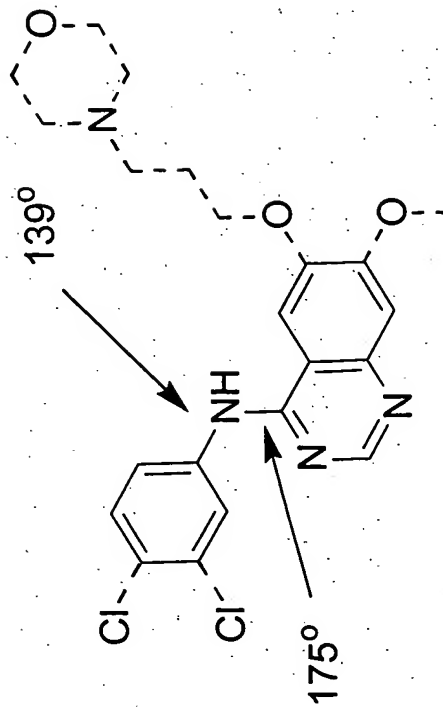


FIG. 8



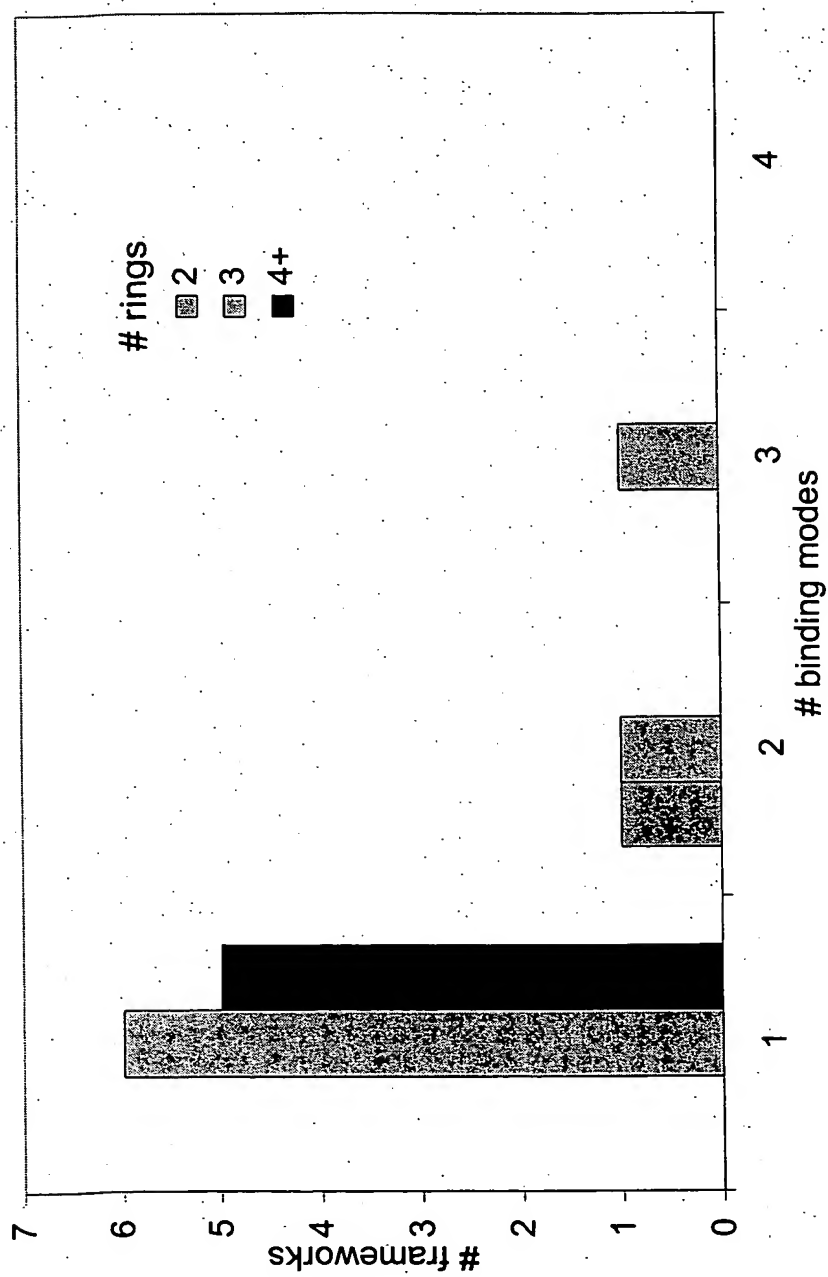


FIG. 9

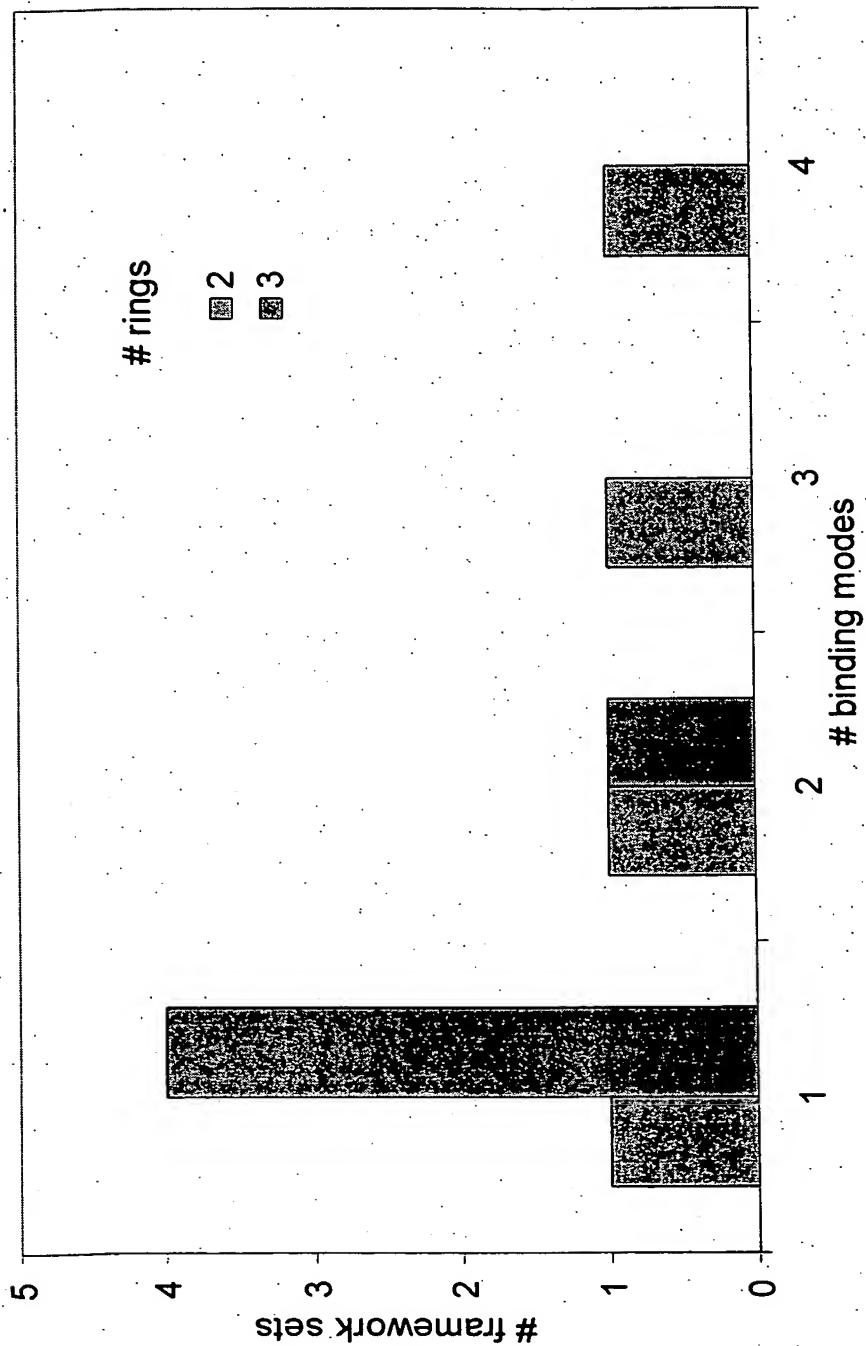


FIG. 10

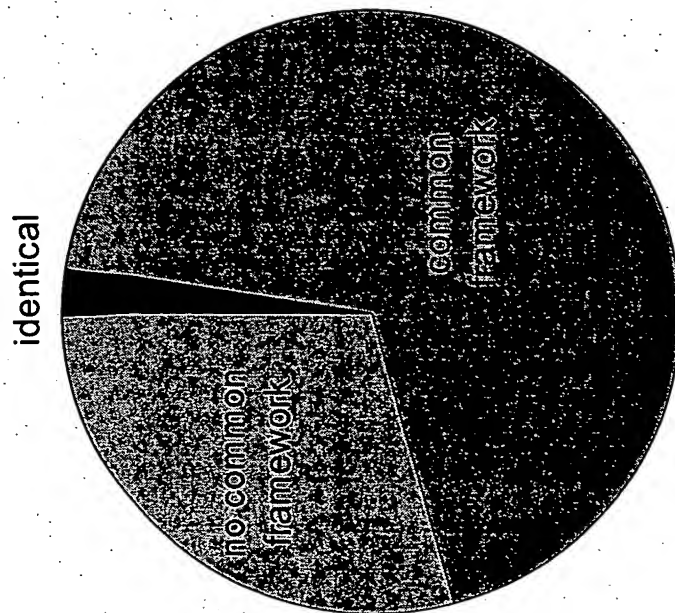


FIG. 11

Applicant(s): Guy Bemis, Paul Caron, Brian Hare
and W. Patrick Walters
MOLECULAR MODELING METHODS

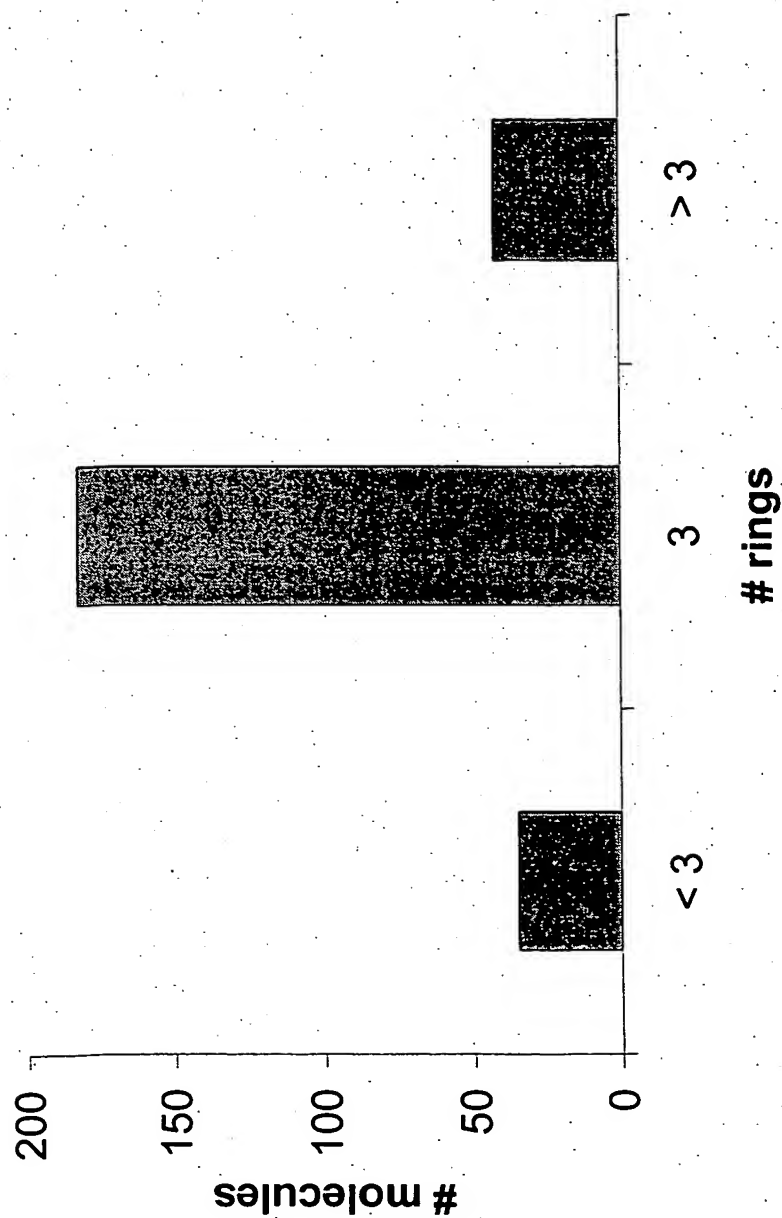
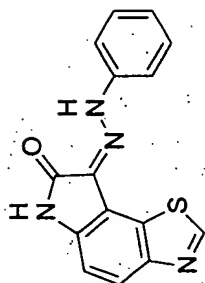
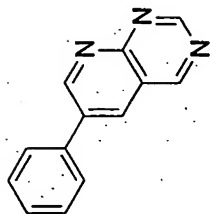


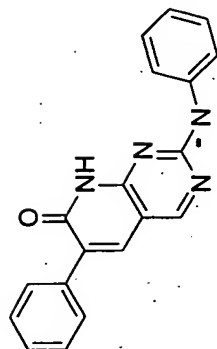
FIG. 12



10



9



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FIG. 13